



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:39 PM GMT

PDB ID : 1LBD
Title : LIGAND-BINDING DOMAIN OF THE HUMAN NUCLEAR RECEPTOR
RXR-ALPHA
Authors : Bourguet, W.; Moras, D.; Structural Proteomics in Europe (SPINE)
Deposited on : 1996-05-22
Resolution : 2.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

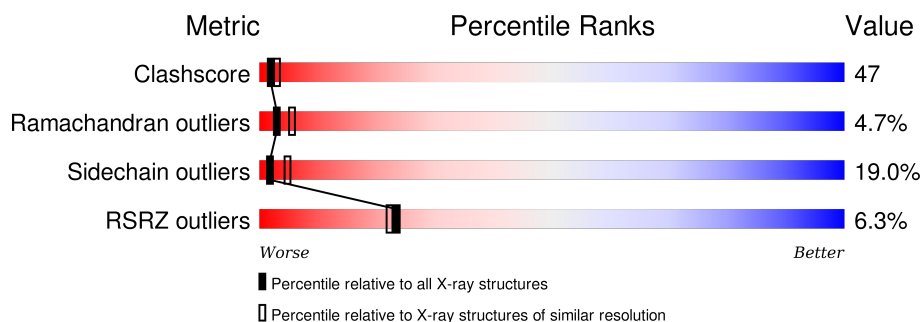
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	282	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1870 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called RETINOID X RECEPTOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	238	1870	1192	320	346	12	0	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	P 63 2 2	Depositor
Cell constants a, b, c, α , β , γ	110.80 Å 110.80 Å 109.90 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	6.00 – 2.70 7.99 – 2.71	Depositor EDS
% Data completeness (in resolution range)	69.4 (6.00-2.70) 79.5 (7.99-2.71)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.90 (at 2.70 Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.230 , 0.323 0.251 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	54.9	Xtriage
Anisotropy	0.270	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	1.30 , 270.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 9164 reflections	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	1870	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.78% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.79	0/1909	1.02	1/2585 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	287	PRO	N-CA-C	5.58	126.61	112.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1870	0	1890	176	0
All	All	1870	0	1890	176	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 47.

All (176) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (\AA)	Clash overlap (\AA)
1:A:414:ARG:O	1:A:418:LEU:HG	1.72	0.89
1:A:372:ALA:HB3	1:A:396:VAL:HG11	1.54	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:357:MET:HG2	1:A:358:ARG:H	1.42	0.82
1:A:315:HIS:HD2	1:A:367:LEU:HD22	1.42	0.82
1:A:424:ALA:O	1:A:428:ILE:HG13	1.82	0.80
1:A:231:PRO:HG2	1:A:234:ARG:HB2	1.62	0.79
1:A:373:ILE:HG23	1:A:393:ARG:HH11	1.47	0.78
1:A:354:VAL:HA	1:A:357:MET:HB3	1.67	0.77
1:A:328:THR:HG22	1:A:330:LEU:HB2	1.66	0.77
1:A:383:LEU:HB2	1:A:386:PRO:HG3	1.67	0.77
1:A:288:HIS:O	1:A:291:GLU:HG3	1.84	0.76
1:A:334:ARG:HA	1:A:346:PHE:CE2	2.22	0.75
1:A:357:MET:HG2	1:A:358:ARG:N	2.03	0.74
1:A:227:ASN:HD21	1:A:232:VAL:HG23	1.51	0.74
1:A:411:GLN:HB3	1:A:412:PRO:HD3	1.70	0.73
1:A:378:PRO:HG2	1:A:390:GLU:HG2	1.71	0.72
1:A:320:VAL:HG11	1:A:331:HIS:CD2	2.25	0.71
1:A:315:HIS:CD2	1:A:367:LEU:HD22	2.24	0.71
1:A:250:VAL:O	1:A:254:MET:HB2	1.94	0.68
1:A:391:ALA:O	1:A:394:GLU:HG2	1.93	0.67
1:A:230:MET:HG3	1:A:395:LYS:HB3	1.76	0.67
1:A:354:VAL:HG13	1:A:357:MET:SD	2.34	0.67
1:A:298:VAL:O	1:A:302:ARG:HG2	1.95	0.66
1:A:356:LYS:HG2	1:A:362:MET:SD	2.35	0.66
1:A:316:ARG:HA	1:A:316:ARG:HE	1.61	0.66
1:A:235:ILE:HD11	1:A:286:ILE:HG23	1.78	0.66
1:A:405:LYS:HE2	1:A:411:GLN:HG3	1.78	0.66
1:A:271:ALA:O	1:A:275:GLN:HG3	1.96	0.65
1:A:235:ILE:HD11	1:A:287:PRO:HD2	1.78	0.65
1:A:305:TRP:CD1	1:A:305:TRP:C	2.71	0.64
1:A:307:GLU:HG2	1:A:425:LEU:HD22	1.79	0.64
1:A:377:ASN:OD1	1:A:379:ASP:HB2	1.99	0.63
1:A:242:VAL:HG22	1:A:278:THR:HG22	1.81	0.62
1:A:334:ARG:HE	1:A:338:HIS:CE1	2.18	0.62
1:A:316:ARG:HD3	1:A:316:ARG:O	1.99	0.61
1:A:315:HIS:O	1:A:318:ILE:HG13	2.00	0.61
1:A:230:MET:CG	1:A:395:LYS:HB3	2.31	0.61
1:A:229:ASP:O	1:A:288:HIS:CE1	2.55	0.60
1:A:358:ARG:NH1	1:A:359:ASP:H	2.00	0.60
1:A:400:LEU:HD23	1:A:415:PHE:CE1	2.38	0.59
1:A:401:GLU:HB2	1:A:415:PHE:CZ	2.38	0.59
1:A:321:LYS:HE3	1:A:322:ASP:OD2	2.02	0.59
1:A:328:THR:CG2	1:A:330:LEU:HB2	2.33	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:460:GLN:NE2	1:A:460:GLN:HA	2.20	0.57
1:A:313:PHE:CD1	1:A:324:ILE:HD13	2.40	0.57
1:A:345:ILE:HD13	1:A:431:LYS:HB3	1.86	0.56
1:A:391:ALA:HA	1:A:394:GLU:OE2	2.05	0.56
1:A:288:HIS:HB2	1:A:392:LEU:HD22	1.88	0.56
1:A:407:LYS:HD3	1:A:408:TYR:CE1	2.41	0.55
1:A:254:MET:HB3	1:A:256:LEU:HD12	1.88	0.55
1:A:358:ARG:HH11	1:A:358:ARG:HG3	1.71	0.55
1:A:289:PHE:CE1	1:A:375:LEU:HD21	2.42	0.55
1:A:296:ASP:O	1:A:300:LEU:HG	2.07	0.55
1:A:358:ARG:HH12	1:A:359:ASP:HB2	1.71	0.55
1:A:316:ARG:CD	1:A:325:LEU:HD23	2.37	0.54
1:A:305:TRP:CG	1:A:306:ASN:N	2.75	0.54
1:A:358:ARG:O	1:A:359:ASP:C	2.46	0.54
1:A:235:ILE:HD12	1:A:286:ILE:HD12	1.89	0.54
1:A:405:LYS:O	1:A:406:HIS:CG	2.61	0.54
1:A:357:MET:SD	1:A:358:ARG:HG2	2.47	0.54
1:A:317:SER:OG	1:A:324:ILE:HA	2.07	0.54
1:A:367:LEU:HG	1:A:367:LEU:O	2.07	0.53
1:A:401:GLU:HA	1:A:404:CYS:SG	2.49	0.53
1:A:281:GLU:OE1	1:A:285:ARG:NH2	2.41	0.53
1:A:270:GLN:O	1:A:273:ASP:HB3	2.08	0.53
1:A:388:GLU:O	1:A:392:LEU:HG	2.09	0.53
1:A:227:ASN:OD1	1:A:231:PRO:HA	2.09	0.53
1:A:321:LYS:HG2	1:A:322:ASP:CG	2.29	0.53
1:A:289:PHE:O	1:A:292:LEU:HB2	2.09	0.53
1:A:358:ARG:HH22	1:A:359:ASP:HB2	1.75	0.52
1:A:334:ARG:HB2	1:A:346:PHE:HE2	1.75	0.52
1:A:235:ILE:CD1	1:A:286:ILE:HG23	2.40	0.52
1:A:236:LEU:HD22	1:A:240:LEU:HD12	1.90	0.52
1:A:378:PRO:CG	1:A:390:GLU:HG2	2.39	0.52
1:A:394:GLU:O	1:A:395:LYS:C	2.49	0.51
1:A:355:SER:O	1:A:360:MET:HB2	2.10	0.51
1:A:285:ARG:CG	1:A:285:ARG:HH11	2.22	0.51
1:A:372:ALA:HB3	1:A:396:VAL:CG1	2.33	0.51
1:A:277:PHE:C	1:A:279:LEU:H	2.14	0.51
1:A:342:VAL:HG11	1:A:437:PHE:HA	1.92	0.50
1:A:345:ILE:HA	1:A:348:ARG:HG3	1.92	0.50
1:A:401:GLU:HA	1:A:415:PHE:CD1	2.47	0.50
1:A:274:LYS:O	1:A:278:THR:OG1	2.30	0.50
1:A:282:TRP:O	1:A:286:ILE:HG12	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:358:ARG:NH1	1:A:359:ASP:HB2	2.28	0.49
1:A:247:GLU:O	1:A:251:GLU:HG3	2.12	0.49
1:A:385:ASN:OD1	1:A:387:ALA:HB3	2.12	0.49
1:A:376:PHE:O	1:A:393:ARG:NE	2.45	0.49
1:A:404:CYS:C	1:A:406:HIS:H	2.16	0.49
1:A:357:MET:O	1:A:358:ARG:C	2.51	0.49
1:A:334:ARG:CA	1:A:346:PHE:CE2	2.94	0.49
1:A:407:LYS:O	1:A:409:PRO:HD3	2.12	0.48
1:A:320:VAL:HG11	1:A:331:HIS:NE2	2.28	0.48
1:A:392:LEU:O	1:A:395:LYS:HB2	2.14	0.48
1:A:309:LEU:O	1:A:313:PHE:CD2	2.67	0.48
1:A:264:PRO:HG3	1:A:450:PHE:HB2	1.95	0.48
1:A:232:VAL:HG13	1:A:365:THR:CG2	2.44	0.48
1:A:320:VAL:HG21	1:A:325:LEU:CD1	2.43	0.48
1:A:316:ARG:HG3	1:A:325:LEU:CB	2.43	0.48
1:A:354:VAL:HG12	1:A:358:ARG:HH11	1.77	0.47
1:A:348:ARG:NH2	1:A:427:SER:OG	2.46	0.47
1:A:357:MET:HG2	1:A:358:ARG:HG2	1.97	0.47
1:A:285:ARG:HG3	1:A:285:ARG:NH1	2.29	0.47
1:A:448:ASP:O	1:A:452:MET:HG3	2.14	0.47
1:A:285:ARG:HG3	1:A:285:ARG:HH11	1.78	0.47
1:A:227:ASN:ND2	1:A:232:VAL:HG23	2.25	0.47
1:A:400:LEU:O	1:A:403:TYR:HB3	2.15	0.47
1:A:239:GLU:O	1:A:242:VAL:HG12	2.14	0.47
1:A:277:PHE:C	1:A:279:LEU:N	2.66	0.47
1:A:305:TRP:O	1:A:305:TRP:CD1	2.68	0.47
1:A:232:VAL:HG13	1:A:365:THR:HG23	1.95	0.46
1:A:342:VAL:CG1	1:A:437:PHE:HD1	2.29	0.46
1:A:242:VAL:HG22	1:A:278:THR:CG2	2.45	0.46
1:A:305:TRP:O	1:A:309:LEU:HB2	2.15	0.46
1:A:314:SER:O	1:A:317:SER:HB2	2.16	0.46
1:A:243:GLU:HG3	1:A:244:PRO:CD	2.45	0.46
1:A:282:TRP:CE2	1:A:286:ILE:HD11	2.50	0.46
1:A:314:SER:O	1:A:353:LEU:CD2	2.63	0.46
1:A:320:VAL:HG21	1:A:325:LEU:HD13	1.98	0.46
1:A:246:THR:O	1:A:250:VAL:HG23	2.16	0.46
1:A:277:PHE:HD1	1:A:277:PHE:HA	1.59	0.46
1:A:316:ARG:HD3	1:A:325:LEU:HD23	1.97	0.45
1:A:254:MET:HB3	1:A:256:LEU:CD1	2.46	0.45
1:A:356:LYS:HB2	1:A:356:LYS:HZ3	1.81	0.45
1:A:358:ARG:NH2	1:A:359:ASP:HB2	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:343:GLY:O	1:A:347:ASP:OD2	2.35	0.45
1:A:260:SER:C	1:A:262:ASN:H	2.18	0.45
1:A:415:PHE:O	1:A:418:LEU:HB2	2.16	0.45
1:A:430:LEU:O	1:A:434:GLU:HG3	2.16	0.45
1:A:407:LYS:HD3	1:A:408:TYR:CD1	2.52	0.45
1:A:435:HIS:O	1:A:436:LEU:HB2	2.17	0.45
1:A:391:ALA:O	1:A:394:GLU:CG	2.64	0.44
1:A:394:GLU:HA	1:A:397:TYR:CE2	2.52	0.44
1:A:330:LEU:HD22	1:A:331:HIS:H	1.82	0.44
1:A:400:LEU:HD23	1:A:415:PHE:HE1	1.80	0.44
1:A:235:ILE:HD11	1:A:287:PRO:CD	2.47	0.44
1:A:369:CYS:CB	1:A:400:LEU:HD13	2.46	0.44
1:A:401:GLU:HB2	1:A:415:PHE:CE1	2.53	0.44
1:A:313:PHE:HE2	1:A:438:PHE:HE1	1.65	0.44
1:A:320:VAL:HG12	1:A:321:LYS:N	2.33	0.44
1:A:302:ARG:HG2	1:A:302:ARG:H	1.38	0.44
1:A:316:ARG:HG3	1:A:325:LEU:HB3	2.00	0.44
1:A:330:LEU:HD22	1:A:331:HIS:N	2.33	0.43
1:A:257:ASN:HA	1:A:258:PRO:HD3	1.85	0.43
1:A:233:GLU:H	1:A:233:GLU:CD	2.22	0.43
1:A:411:GLN:CB	1:A:412:PRO:HD3	2.46	0.43
1:A:422:LEU:N	1:A:423:PRO:HD2	2.33	0.43
1:A:289:PHE:O	1:A:292:LEU:N	2.52	0.43
1:A:282:TRP:CD2	1:A:371:ARG:NH1	2.87	0.42
1:A:370:LEU:O	1:A:373:ILE:HB	2.19	0.42
1:A:316:ARG:CD	1:A:316:ARG:O	2.68	0.42
1:A:240:LEU:HA	1:A:240:LEU:HD23	1.86	0.42
1:A:342:VAL:HG11	1:A:437:PHE:HD1	1.85	0.42
1:A:276:LEU:O	1:A:279:LEU:CB	2.68	0.42
1:A:373:ILE:HD11	1:A:397:TYR:HB3	2.01	0.42
1:A:229:ASP:O	1:A:288:HIS:HE1	2.00	0.41
1:A:439:PHE:O	1:A:439:PHE:CD2	2.73	0.41
1:A:235:ILE:HD13	1:A:235:ILE:HA	1.83	0.41
1:A:327:ALA:C	1:A:329:GLY:H	2.24	0.41
1:A:243:GLU:HG3	1:A:244:PRO:HD2	2.02	0.41
1:A:376:PHE:O	1:A:393:ARG:HB2	2.20	0.41
1:A:246:THR:O	1:A:246:THR:HG22	2.20	0.41
1:A:275:GLN:O	1:A:276:LEU:C	2.59	0.41
1:A:363:ASP:OD1	1:A:366:GLU:HG3	2.21	0.41
1:A:411:GLN:HB3	1:A:412:PRO:CD	2.46	0.41
1:A:334:ARG:O	1:A:334:ARG:HG2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:295:ASP:HA	1:A:298:VAL:CG1	2.50	0.41
1:A:358:ARG:NH1	1:A:358:ARG:HG3	2.35	0.41
1:A:236:LEU:HG	1:A:365:THR:OG1	2.21	0.41
1:A:279:LEU:HD13	1:A:309:LEU:HD23	2.03	0.41
1:A:414:ARG:HD2	1:A:414:ARG:HA	1.71	0.40
1:A:357:MET:O	1:A:359:ASP:N	2.54	0.40
1:A:232:VAL:CG1	1:A:365:THR:HG21	2.51	0.40
1:A:350:LEU:O	1:A:354:VAL:CG2	2.70	0.40
1:A:227:ASN:HD21	1:A:232:VAL:CG2	2.28	0.40
1:A:360:MET:O	1:A:361:GLN:HB2	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	236/282 (84%)	198 (84%)	27 (11%)	11 (5%)	3 5

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	342	VAL
1	A	358	ARG
1	A	361	GLN
1	A	260	SER
1	A	258	PRO
1	A	289	PHE
1	A	411	GLN
1	A	461	MET
1	A	328	THR
1	A	406	HIS
1	A	408	TYR

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	205/244 (84%)	166 (81%)	39 (19%)	2 5

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	227	ASN
1	A	228	GLU
1	A	236	LEU
1	A	237	GLU
1	A	247	GLU
1	A	248	THR
1	A	253	ASN
1	A	257	ASN
1	A	270	GLN
1	A	277	PHE
1	A	278	THR
1	A	285	ARG
1	A	287	PRO
1	A	290	SER
1	A	294	LEU
1	A	302	ARG
1	A	305	TRP
1	A	309	LEU
1	A	312	SER
1	A	315	HIS
1	A	316	ARG
1	A	328	THR
1	A	330	LEU
1	A	334	ARG
1	A	335	ASN
1	A	350	LEU
1	A	352	GLU
1	A	354	VAL
1	A	358	ARG
1	A	369	CYS

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Mol	Chain	Res	Type
1	A	381	LYS
1	A	384	SER
1	A	390	GLU
1	A	425	LEU
1	A	427	SER
1	A	441	LEU
1	A	442	ILE
1	A	455	LEU
1	A	460	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	288	HIS
1	A	315	HIS
1	A	338	HIS
1	A	460	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	238/282 (84%)	-0.00	15 (6%) 23 22	20, 36, 66, 83	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	461	MET	7.3
1	A	260	SER	6.7
1	A	413	GLY	4.7
1	A	406	HIS	3.5
1	A	412	PRO	3.4
1	A	359	ASP	3.4
1	A	460	GLN	3.0
1	A	462	THR	2.8
1	A	262	ASN	2.7
1	A	409	PRO	2.4
1	A	361	GLN	2.4
1	A	259	SER	2.3
1	A	225	SER	2.3
1	A	411	GLN	2.2
1	A	458	PRO	2.1

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.